

COPY

THE MERCK INDEX

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CHEMICALS, DRUGS, AND BIOLOGICALS

TWELFTH EDITION

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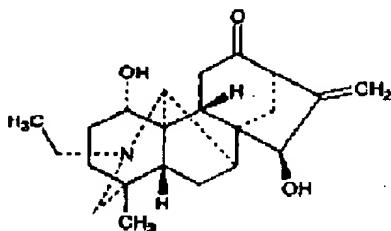
Sorbic Alcohol

8870

THERAP CAT: Growth stimulant.

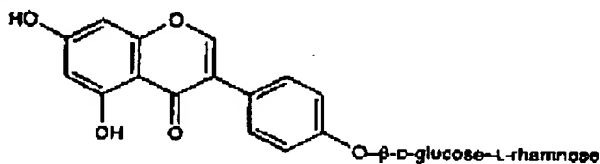
THERAP CAT (VET): Growth stimulant. Bovine somatotropin as galactopoietic.

8865. Songorine. (1 α ,15 β)-21-Ethyl-1,15-dihydroxy-4-methyl-16-methylene-7,20-cyclooctan-12-one; napellonine; songorine. $C_{27}H_{31}NO_3$; mol wt 357.49. C 73.92%, H 8.74%, N 3.92%, O 13.43%. From *Aconitum songoricum* Popov, *Ranunculaceae*: Yunusov, *J. Gen. Chem. USSR* 18, 515 (1948); Kuzovkov, *Ibid.* 23, 504 (1953); 25, 2006 (1955). Identity with napellonine: Kuzovkov, *Zh. Obshch. Khim.* 28, 2283 (1958); 29, 1728 (1959). Structure: Sugawara, *Chem. Pharm. Bull.* 9, 889, 897 (1961). Absolute configuration: Okamoto *et al.*, *ibid.* 13, 1270 (1965). Synthesis of the aromatic intermediate: Wiesner *et al.*, *Can. J. Chem.* 51, 3978 (1973). Pharmacology: Sadritdinov, *Farmakol. Akk. No.* 312 (1965), *C.A.* 66, 93772d (1967). Mass spectra data: Yunusov *et al.*, *Khim. Priir. Soedn.* 6, 101 (1970). *C.A.* 73, 131178u (1970).



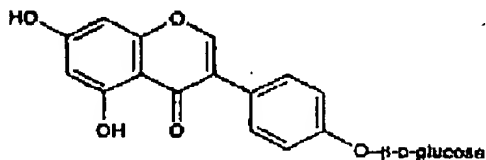
Crystals, mp 201-202°. $[\alpha]_D^{20} -135.4^\circ$. uv max: 290 nm ($\log \epsilon$ 2.6). LD_{50} in mice: 142.5 mg/kg. Hydrochloride, crystals, mp 257-258°. $[\alpha]_D^{20} -114^\circ$ ($c = 2$ in water).

8866. Sopharabloside. 3-[4-[(2-O-(6-Deoxy- α -L-mannopyranosyl)- β -D-glucopyranosyl)oxy]phenyl]-5,7-dihydroxy-4H-1-benzopyran-4-one; genistein-4'-glucosidorrhamnoside. $C_{27}H_{30}O_{14}$; mol wt 578.53. C 56.06%, H 5.23%, O 38.72%. From fruits of *Sophora japonica* L., *Leguminosae*. Isola and structure: Zemplén, Bognár, *Ber.* 75B, 482 (1942). The bioside is not identical with rutinose.



The anhydr substance mp 248° (slight decompn). $[\alpha]_D^{20} -73^\circ$ (0.27 g in 10 ml pyridine). Freely sol in pyridine; sol in hot alcohol, hot acetone; slightly sol in boiling water. The alcoholic soln gives a purple color with ferric chloride. Trihydrate, needles from dil alcohol, mp 156-160°. The water of crystn can be removed by drying at 100° over P_2O_5 in *vacuo* for 12 hours.

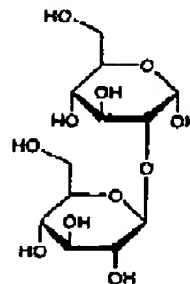
8867. Sophoricoside. 3-[4-(β -D-Glucopyranosyloxy)-phenyl]-5,7-dihydroxy-4H-1-benzopyran-4-one; 4',5,7-trihydroxyisoflavone-4'-D-glucoside; genistein-4'-glucoside. $C_{27}H_{30}O_{14}$; mol wt 432.38. C 58.33%, H 4.66%, O 37.00%. From the green pods of *Sophora japonica* L., *Leguminosae*: Charaux, Rabate, *Bull. Soc. Chim. Biol.* 20, 454 (1938). Structure: Zemplén *et al.*, *Ber.* 76, 267 (1943); Bognár, *C.A.* 46, 8104h (1952). Synthesis: Bognár, Szabo, *Acta Chim. Acad. Sci. Hung.* 4, 383 (1954); *Chem. & Ind. (London)* 1954, 518. Hydrolyzed by emulsin or by dil acids.



Crystals from alcohol, mp 298°. $[\alpha]_D^{20} -47^\circ$ (pyridine). $[\alpha]_D^{20} -32^\circ$ (10% aq pyridine). uv max (abs ethanol): 262

nm. Sparingly sol in water, alc, acetic acid; more sol in hot alc, hot acetic acid; sol in pyridine, dil alkalies; practically insol in ethyl acetate, acetone. Ferric chloride gives the color of red wine to alcoholic solns which turn orange after addition of a few drops of Na-carbonate soln.

8868. Sophorose. 2-O- β -D-Glucopyranosyl- α -D-glucose. $C_{12}H_{22}O_{11}$; mol wt 342.30. C 42.11%, H 6.48%, O 51.41%. From pods of *Sophora japonica* L., *Leguminosae*: Rebatié, *Bull. Soc. Chim. France* 7, 565 (1940); Clancy, *J. Chem. Soc.* 1960, 4213; Clancy in *Methods in Carbohydrate Chemistry* vol. I, R. L. Whistler, M. L. Wolfrom, Eds. (Academic Press, New York, 1962) pp 345-349. Structure and synthesis: Coxon, Fletcher, *J. Org. Chem.* 26, 2892 (1961); Koeppen, *Carbohydr. Res.* 7, 410 (1968). Crystal structure: J. Ohanessian *et al.*, *Acta Crystallogr.* B34, 3666 (1978).



Monohydrate, needles from 80% aq methanol, mp 196-198°. $[\alpha]_D^{20} +19^\circ$ ($c = 1.2$ in water). Octa-O-acetyl- β -sophorose, $C_{22}H_{38}O_{16}$, needles from ethanol, mp 193-194°. $[\alpha]_D^{20} -3.2^\circ$ ($c \approx 2.5$ in chloroform).

8869. Sorbic Acid. (E,E)-2,4-Hexadienoic acid; 2-propenylacrylic acid. $C_6H_8O_2$; mol wt 112.13. C 64.27%, H 7.19%, O 28.54%. $CH_3CH=CHCH=CHCOOH$. May be obtained from berries of the mountain ash, *Sorbus aucuparia* L., *Rosaceae* where it occurs as the lactone, called parasorbic acid: Hofmann, *Ann.* 110, 129 (1859). Synthesis by condensing crotonaldehyde and malonic acid in pyridine soln: Doebner, *Ber.* 33, 2140 (1900); Allen, Van Allan, *Org. Syn. coll. vol. III*, 783 (1955); by condensing crotonaldehyde and ketene in the presence of boron trifluoride: Hagemeyer, Jr., *Ind. Eng. Chem.* 41, 768 (1949). Prepn from 1,1,3,5-tetraalkoxyhexane: Parker, MacLean, U.S. pat. 2,921,090 (1960 to Celanese). Additional syntheses: Fernholz, Mundlos, Ger. pat. 1,049,852; U.S. pat. 3,021,365 (1959, 1962 both to Hoechst). Prepn of sodium salt: Horn, Fernholz, Ger. pat. 1,045,390 (1958 to Hoechst); of calcium salt: C. M. Gooding, U.S. pat. 3,139,378 (1964 to Corn Products Co.). Purification: Fernholz, Ger. pat. 1,044,803 (1958 to Hoechst). The *trans,trans*-isomer is usually obtained and is the commercial product. Toxicity study: Smyth, Carpenter, *J. Ind. Hyg. Toxicol.* 30, 63 (1948).

Needles from water, mp 134.5°. Should be stored at temps below 40°, bp 228° (dec). Vapor pressure at 20° < 0.01 mm, at 143° 50 mm. Flash pt 260°F (127°C). pK (25°) = 4.76. Soly in water at 30° 0.25%, at 100° 3.8%, in propylene glycol at 20° 5.5%, in abs ethanol or methanol 12.90%, in 20% ethanol 0.29%, in glacial acetic acid 11.5%, in acetone 9.2%, in benzene 2.3%, in carbon tetrachloride 1.3%, in cyclohexane 0.28%, in dioxane 11.0%, in glycerol 0.31%, in isopropanol 8.4%, in isopropyl ether 2.7%, in methyl acetate 6.1%, in toluene 1.9%. LD_{50} orally in rats: 7.36 g/kg (Smyth, Carpenter).

USE: Mold and yeast inhibitor. Fungistatic agent for foods, especially cheeses. To improve the characteristics of drying oils. In alkyl type coatings to improve gloss. To improve milling characteristics of cold rubber. See also Potassium Sorbate.

8870. Sorbic Alcohol. 2,4-Hexadien-1-ol; 1-hydroxy-2,4-hexadiene; hexadenol; Hexene-Ol; Hexakose. $C_6H_{10}O$; mol wt 98.14. C 73.43%, H 10.27%, O 16.30%. $CH_3CH=CHCH=CHCH_2OH$. Prepd from sorbic aldehyde by means of aluminum isopropylate in isopropanol: Reichstein *et al.*, *Helv. Chim. Acta* 15, 264 (1932).